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Problem Set 2

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Exercise 1 : Carrier density in a semiconductor

Consider electrons in the conduction band of a semiconductor with anisotropic dispersion relation

$$\epsilon(\vec{k}) = \epsilon_c + \frac{\hbar^2}{2}\left(\frac{k_x^2}{m_x} + \frac{k_y^2}{m_y} + \frac{k_z^2}{m_z}\right).$$

a) Show that the dispersion relation can be written as

$$\epsilon(\vec{q}) = \epsilon_c + \frac{\hbar^2}{2m_c^*}(q_x^2 + q_y^2 + q_z^2)$$

with the effective mass $m_c^* = (m_x m_y m_z)^{1/3}$. Express the components q_i ($i = \{x, y, z\}$) of the momentum $\vec{q}$ as functions of k_i, m_i and m_c^*.

$$\epsilon(\vec{k}) = \epsilon_c + \frac{\hbar^2}{2}\left(\frac{k_x^2}{m_x} + \frac{k_y^2}{m_y} + \frac{k_z^2}{m_z}\right)$$

$$= \epsilon_c + \frac{\hbar^2}{2m_c^*}\left(m_c^*\frac{k_x^2}{m_x} + m_c^*\frac{k_y^2}{m_y} + m_c^*\frac{k_z^2}{m_z}\right)$$

$$= \epsilon_c + \frac{\hbar^2}{2m_c^*}(q_x^2 + q_y^2 + q_z^2)$$

Meaning,

$$q_i = k_i\sqrt{\frac{m_c^*}{m_i}}$$

b) Determine the density of states $g_c(\epsilon)$ in such a conduction band. Compare to the free-electron density of states discussed in TD1.

Number of states under E,

$$q_x^2 + q_y^2 + q_z^2 \leq \frac{2m_c^*(\epsilon - \epsilon_c)}{\hbar^2}$$

Thus,

$$N(\epsilon) = \frac{4}{3}\pi\left(\sqrt{\frac{2m_c^*}{\hbar^2}}\sqrt{|\epsilon - \epsilon_c|}\right)^3\frac{V}{(2\pi)^3}$$

So the density of states,

$$g(\epsilon) = \frac{1}{V}\frac{\mathrm{d}N(E)}{\mathrm{d}E}$$

$$= \frac{4}{3}\frac{\pi}{(2\pi)^3}\left(\frac{2m_c^*}{\hbar^2}\right)^{3/2}\frac{3}{2}|\epsilon - \epsilon_c|^{1/2}$$

$$= \frac{1}{(2\pi)^2}\left(\frac{2m_c^*}{\hbar^2}\right)^{3/2}\sqrt{|\epsilon - \epsilon_c|}$$

This is valid for $\epsilon > \epsilon_c$, it is 0 otherwise.

c) Express the finite-temperature carrier density $n_c(T)$ in terms of the density of states $g_c(\epsilon)$ and as a function of the chemical potential μ and the temperature T. Show that for $\epsilon_c - \mu \gg k_B T$, the carrier density can be approximated by $n_c(T) = N_c(T)e^{-(\epsilon_c - \mu)/k_B T}$ with

$$N_c(T) = \int_{\epsilon_c}^{+\infty} d\epsilon \, g_c(\epsilon) e^{-(\epsilon - \epsilon_c)/k_B T}.$$

$$n_c(T) = \int_{\epsilon_c}^{+\infty} d\epsilon \, g_c(\epsilon) \frac{1}{e^{(\epsilon - \mu)/k_B T} + 1}$$

With the condition that $\epsilon_c - \mu \gg k_B T$, and for $\epsilon > \epsilon_c$,

$$\frac{1}{e^{(\epsilon - \mu)/k_B T} + 1} \simeq e^{-(\epsilon - \mu)/k_B T}$$

Thus,

$$\begin{aligned}
n_c(T) &= \int_{\epsilon_c}^{+\infty} d\epsilon \, g_c(\epsilon) \frac{1}{e^{(\epsilon - \mu)/k_B T} + 1} \\
&\approx \int_{\epsilon_c}^{+\infty} d\epsilon \, g_c(\epsilon) e^{-(\epsilon - \mu)/k_B T} \\
&= \left\{ \int_{\epsilon_c}^{+\infty} d\epsilon \, g_c(\epsilon) e^{-(\epsilon - \epsilon_c)/k_B T} \right\} e^{-(\epsilon_c - \mu)/k_B T} \\
&= N_c(T) e^{-(\epsilon_c - \mu)/k_B T}
\end{aligned}$$

d) Apply the same reasoning to holes in the valence band, and derive the approximation for the hole density $p_v = P_v(T)e^{-(\mu - \epsilon_v)/k_B T}$. Give the expression for $P_v(T)$ and the condition for the validity of the approximation.

$$p_v(T) = \int_{-\infty}^{\epsilon_v} d\epsilon \, g_v(\epsilon) \left(1 - \frac{1}{e^{(\epsilon - \mu)/k_B T} + 1} \right)$$

With the condition that $\mu - \epsilon_v \gg k_B T$ and for $\epsilon < \epsilon_v$,

$$\frac{1}{e^{(\mu - \epsilon)/k_B T} + 1} \simeq e^{-(\mu - \epsilon)/k_B T}$$

Thus,

$$p_v(T) = \int_{-\infty}^{\epsilon_v} d\epsilon g_v(\epsilon) \left(1 - \frac{1}{e^{(\epsilon-\mu)/k_B T} + 1} \right)$$

$$= \int_{-\infty}^{\epsilon_v} d\epsilon g_v(\epsilon) \frac{1}{e^{(\mu-\epsilon)/k_B T} + 1}$$

$$= \int_{-\infty}^{\epsilon_v} d\epsilon g_v(\epsilon) e^{-(\mu-\epsilon)/k_B T}$$

$$= \int_{-\infty}^{\epsilon_v} d\epsilon g_v(\epsilon) e^{(\mu-\epsilon_v)/k_B T} e^{-(\mu-\epsilon)/k_B T} e^{-(\mu-\epsilon_v)/k_B T}$$

$$= \int_{-\infty}^{\epsilon_v} d\epsilon g_v(\epsilon) e^{-(\epsilon_v-\epsilon)/k_B T} e^{-(\mu-\epsilon_v)/k_B T}$$

$$= \left\{ \int_{-\infty}^{\epsilon_v} d\epsilon g_v(\epsilon) e^{-(\epsilon_v-\epsilon)/k_B T} \right\} e^{-(\mu-\epsilon_v)/k_B T}$$

$$= P_v(T) e^{-(\mu-\epsilon_v)/k_B T}$$

e) Show that within the above approximations, the product of n_c and p_v is independent of the chemical potential. Express it in terms of the energy gap $E_g = \epsilon_c - \epsilon_v$ of the semiconductor.

$$n_c(T)p_v(T) = N_c(T) e^{-(\epsilon_c-\mu)/k_B T} P_v(T) e^{-(\mu-\epsilon_v)/k_B T}$$

$$= N_c(T) P_v(T) e^{-(\epsilon_c-\epsilon_v)/k_B T}$$

$$= N_c(T) P_v(T) e^{-E_g/k_B T}$$

Exercise 2 : Intrinsic semiconductor

a) Explain the meaning of "intrinsic semiconductor".

If the crystal is pure and the impurities effect is making negligible contribution to the charge carries, we speaks about *intrinsic semiconductor.*

b) Assume low enough temperature and use the approximate results for the carrier and hole densities of Exercise 1. Express the intrinsic carrier density $n_i = n_c = p_v$ in terms of the energy gap.

$$n_i = (n_c(T)p_v(T))^{1/2}$$

Thus,

$$n_i(T) = [N_c(T)P_v(T)]^{1/2}e^{-E_g/2k_BT}$$

c) Derive an expression for the chemical potential μ from the condition of charge conservation (equal number of electrons in the conduction band and holes in the valence band).

$$\begin{cases} n_c(T) = N_c(T)e^{-(\epsilon_c-\mu)/k_BT} \\ p_v(T) = P_v(T)e^{-(\mu-\epsilon_v)/k_BT} \end{cases}$$

$$n_c(T) = p_v(T) \implies \frac{P_v}{N_c} = e^{-(\epsilon_c-\mu)/k_BT}e^{(\mu-\epsilon_v)/k_BT} = e^{2\mu/k_BT}e^{-(\epsilon_c+\epsilon_v)/k_BT}$$

Thus,

$$e^{2\mu/k_BT} = \frac{P_v}{N_c}e^{+(\epsilon_c+\epsilon_v)/k_BT}$$

$$\begin{aligned} \mu &= \frac{1}{2}k_BT\ln\left[\frac{P_v}{N_c}e^{+(\epsilon_c+\epsilon_v)/k_BT}\right] \\ &= \frac{1}{2}(\epsilon_c+\epsilon_v)\frac{1}{2}k_BT\ln\left(\frac{P_v}{N_c}\right) \\ &= \frac{1}{2}(E_g+\epsilon_v+\epsilon_v)+\frac{1}{2}k_BT\ln\left(\frac{P_v}{N_c}\right) \\ &= \epsilon_v+\frac{E_g}{2}+\frac{1}{2}k_BT\ln\left(\frac{P_v}{N_c}\right) \end{aligned}$$

d) Take an energy gap $E_g = 0.6$ eV, and an effective mass m_c^* in the conduction band which is three times the effective mass m_v^* in the valence band. Calculate the temperature for which the chemical potential μ is situated at $\epsilon_v + E_g/3$.

$$\frac{P_v}{N_c} \propto \left(\frac{m_v^*}{m_c^*}\right)^{3/2} = \left(\frac{1}{3}\right)^{3/2}$$

We seek T such that,

$$\mu = \epsilon_v + \frac{E_g}{3} = \epsilon_v + \frac{E_g}{2} + \frac{1}{2}k_B T \ln\left(\frac{P_v}{N_c}\right)$$

Which is equivalent to seek,

$$-\frac{E_g}{6} = -\frac{1}{2}k_B T \frac{3}{2}\ln(3)$$

Thus,

$$T = \frac{2E_g}{9\ln 3}\frac{1}{k_B}$$

$$T = \frac{\frac{3}{5}2}{9k_B \ln 3} \times 1.605 \times 10^{-19} = \frac{2}{15\ln 3}\frac{1}{1.381 \times 10^{-23}} \times 1.605 \times 10^{-19} \approx 1410.51 \text{ K}$$

Exercise 3 : Doped semiconductors

The semiconductor InSb has a gap $Eg = 0.18$ eV. The dielectric constant of the material is $\epsilon = \epsilon_0 \epsilon_r$ with $\epsilon_r = 17$). The effective mass is $m_c^* = 0.014 m_0$, where m_0 is the free electron mass. Some of the In atoms (group III of the periodic system) are replaced by Si donor atoms (group IV), with a donor dopant density $n_d = 10^{18}$ cm^{-3}. Let us treat a donor atom as a positively charged Si atom with a weakly bound electron in a hydrogen-like state.

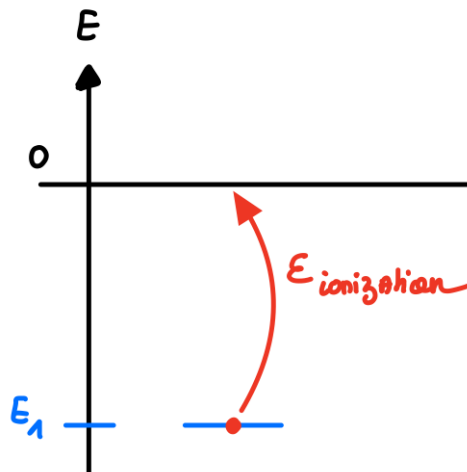a) The energy levels of a hydrogen atom are given by

$$E_n = -\frac{m_0 e^4}{8\epsilon_0^2 h^2} \frac{1}{n^2}.$$

Calculate the ground state energy E_1 of the hydrogen atom in eV and determine the ionization energy (Rydberg constant Ry).
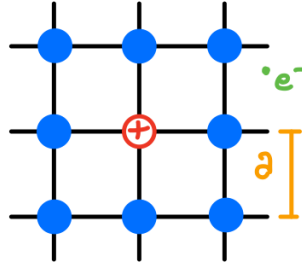
$$E_1 = -\frac{m_0 e^4}{8\epsilon_0 h^2} \simeq -13.6 \text{ eV}$$

Ionization energy is the energy you need to add to make the energy go to 0, thus,

$$E_{\text{Ionization}} + E_1 = 0 \implies E_{\text{Ionization}} = \frac{m_0 e^4}{8\epsilon_0^2 h^2} = 13.6 \text{ eV} > 0$$

b) In analogy with the previous case, express the ionization energy of a donor in a semiconductor in units of Ry and calculate its value for Si donors in InSb.

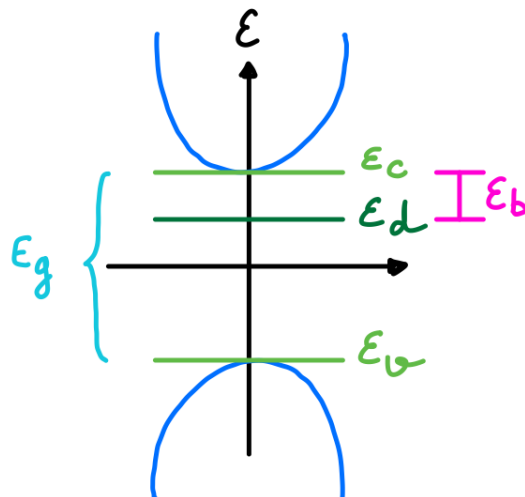The electron is "far" from the positive site, far in comparison to the lattice constant size,

$$E_{\text{binding}} = \frac{m^*}{m_0} \frac{1}{\epsilon_r^2} E_1$$

This $1/\epsilon_r^2$ is here because of the modification of the dielectric constant : $\epsilon_0 \to \epsilon = \epsilon_0 \epsilon_r$. Thus,

$$E_{\text{binding}} = \frac{0.014}{17^2} E_1 = 4.8 \times 10^{-5} E_1 = -0.6 \text{ meV}$$

And so we get ionization energy,

$$\epsilon_{\text{ionization}} = \epsilon_c - \epsilon_b = -E_{\text{binding}} = 0.6 \text{ meV}$$

c) Compare the ionization energy to the thermal energy at room temperature and to the energy gap of the semiconductor.

At $T = 300$ K, $k_B T \simeq 26$ meV, and thus,

$$\frac{\epsilon_{\text{ionization}}}{k_B T} \simeq \frac{0.6}{26} \simeq \frac{1}{40}$$

Meaning that

$$\epsilon_{\text{ionization}} \ll k_B T < E_g$$

d) The typical distance between the electron and the nucleus in a hydrogen atom is given by the Bohr radius

$$a_0 = \frac{h^2 \epsilon_0}{\pi m_0 e^2} \approx 52.92 \text{ pm.}$$

Estimate the distance between a Si donor atom and the weakly bound electron.

$$r_0 = \frac{m}{m^*} \epsilon \frac{\hbar^2}{me^2} = \frac{17}{0.014} a_0 = 1214 a_0 \gg a_0 \approx 642 \text{ Å}$$

Thus, $r_0 \gg a_0$.

e) Estimate the critical dopant concentration above which the distance between dopants is small enough to allow for the hopping of electrons between neighboring dopants. At what temperatures is this effect expected to be important?

If the distance d is of the order of r_0, the wavefunctions can be overlapped. Thus,

$$n_d = \frac{N_d}{V} \propto \frac{1}{d^2}$$

So we get $n_d = 3.8 \times 10^{15}$ cm^{-3}, and in the sheet we got $n_d = 10^{18}$ cm^{-3} that is greater than this one, meaning that the distance d is lower than r_0, thus there is an overlapping of the wavefunctions.

We saw that

$$\frac{\epsilon_{\text{ionization}}}{k_B T} \simeq \frac{0.6}{26} \simeq \frac{1}{40}$$

Thus,

$$k_B T_{\text{room}} = 40 \epsilon_{\text{ionization}}$$

Thus,

$$\epsilon_{\text{ionization}} = \frac{k_B T_{\text{room}}}{40} = k_B T \Big|_{T=7.5 \text{ K}}$$

Thus, as long as we are a temperature greater than 7.5 K, the effect are negligible.

Exercise 4 : Some simple calculations

a) Estimate the slope of the temperature dependence of the intrinsic carrier concentration in the vicinity of room temperature, for the semiconductors InAs, Si and GaAs. Intrinsic carrier concentrations at room temperature (300 K) are for InAs : 8.6×10^{14} cm^{-3}, Si : 1.0×10^{10} cm^{-3}, GaAs : 1.8×10^{6} cm^{-3}. Energy gaps : InAs : 0.36 eV, Si : 1.1 eV, GaAs : 1.43 eV.

$$n_i(T) = [N_c(T)P_v(T)]^{1/2}e^{-E_g/2k_BT} = \frac{1}{4}\left(\frac{2k_BT}{\pi\hbar^2}\right)^{3/2}(m_c^*m_v^*)^{3/4}e^{-E_g/2k_BT}$$

To get the slope, we just have to calculate the derivative,

$$\frac{\mathrm{d}n_i}{\mathrm{d}T} = \underbrace{\frac{1}{4}(m_c^*m_v^*)^{3/4}\left(\frac{2k_B}{\pi\hbar^2}\right)^{3/2}}_{=A}\left(\frac{3}{2}T^{1/2}e^{-E_g/2k_BT} + T^{3/2}\frac{E_g}{2k_BT^2}e^{-E_g/2k_BT}\right)$$

$$= \frac{3}{2}AT^{1/2}e^{-E_g/2k_BT} + n_i\frac{E_g}{2k_BT^2}$$

$$= \left(3 + \frac{E_g}{k_BT}\right)\frac{n_i}{2T}$$

For InAs :

$$\left.\frac{\mathrm{d}n_i}{\mathrm{d}T}\right|_{300\text{ K}} = 0.24 \times 10^{14} \text{ cm}^{-3}.\text{K}^{-1}$$

For Si :

$$\left.\frac{\mathrm{d}n_i}{\mathrm{d}T}\right|_{300\text{ K}} = 0.07 \times 10^{10} \text{ cm}^{-3}.\text{K}^{-1}$$

For GaAs :

$$\left.\frac{\mathrm{d}n_i}{\mathrm{d}T}\right|_{300\text{ K}} = 0.17 \text{ cm}^{-3}.\text{K}^{-1}$$

b) Take the case of doped silicon with an electron density in the conduction band $n_c = 10^{16}$ cm^{-3} at $T = 300$ K. Using the value $N_c = 7.28 \times 10^{19}$ cm^{-3} at $T = 300$ K, determine the value of the chemical potential with respect to the bottom of the conduction band ϵ_c.

$$n_c(T) = N_c(T)e^{-(\epsilon_c-\mu)/k_BT}$$

Thus,

$$\frac{n_c}{N_c} = e^{-(\epsilon_c - \mu)/k_B T}$$

Meaning,

$$-k_B T \ln\left(\frac{n_c}{N_c}\right) = \epsilon_c - \mu$$

So we get,

$$\mu = \epsilon_c + k_B T \ln\left(\frac{n_c}{N_c}\right)$$
$$= \epsilon_c + 300 k_B \ln\left(\frac{10^{16}}{7.28 \times 10^{19}}\right)$$
$$= \epsilon_c + 300 k_B (-8.89)$$
$$= \epsilon_c - 0.2299 \text{ eV}$$

c) Calculate the mean distance between dopants in silicon for dopant concentrations of (1) 10^{16} cm^{-3}; (2) 10^{18} cm^{-3}; and (3) 10^{20} cm^{-3}.

(1) $= 46$ nm.

(2) $= 10$ nm.

(3) $= 2.2$ nm.